Fakultät für Naturwissenschaften

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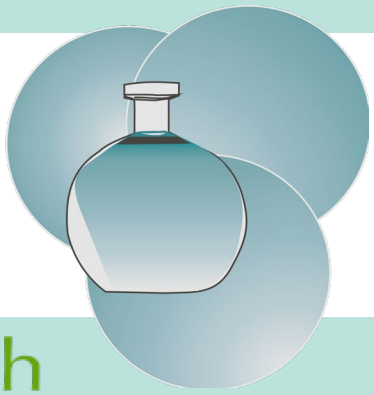

lädt ein

gemeinsam mit der Gesellschaft Deutscher Chemiker zum

Vortrag

von Herrn

Prof. Dietmar Stalke

Institut für Anorganische Chemie
Universität Göttingen

Gesellschaft Deutscher Chemiker

“Basic chemical concepts challenged by experimental charge”

am: 06. Februar 2025

um: 16:00 Uhr

wo: im Raum 1/232

Die kleine Kaffeerunde vor dem Vortrag beginnt um 15:30 Uhr im Raum 1/232.
Das Mitbringen von eigenen Trinkgefäßen ist erwünscht.

Gäste sind herzlich willkommen!

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Basic chemical concepts challenged by experimental charge density

From the knowledge of the distances at the atomic level and the arrangement in the solid phase many properties, both at the molecular and materials scale, can be deduced. However, the most basic concept, the chemical bond and reactivity, is still vigorously discussed. Still there is room for interpretation, because single crystal structural analyses based on the independent atom model only provides the positions of the centroids of the atoms and the distances between the atoms. In the electron density maps there are no lines or dashes defining or even indicating the chemical bond and the nature of the bonding remains a matter of interpretation based on a bonding model. Hence the anecdote that a bond is where the chemist draws the line remains valid to a certain extent. Most of our understanding of the chemical bond is still deduced from the distances and angles, which are determined as a result of the crystallographic analysis and reactivity is introduced on this basis.1 Various topics are addressed in the talk and connected to reactivity:

1) BnSe$^{\bullet}$ *vs*. BnSeSe$^{\bullet}$ radical formation upon irradiation.[2]
2) Straight *vs*. bent Cp*$_2$Si.[3]
3) Chalcogen···hydride bonding in Si–H activation.[4]

3) S=N *vs.* S$^{\delta}$ +–N$^{\delta}$– bonding and consequences to e. g. single-molecule magnets.[5]

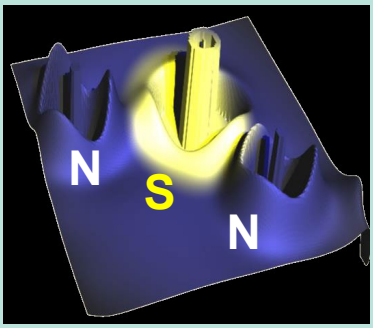

Figure 1. S=N *vs.* S$^{\delta}$ +–N$^{\delta}$

References

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2. C. J. Schürmann, T. L. Teuteberg, A. C. Stückl, P. N. Ruth, F. Hecker, R. Herbst-Irmer, R. A. Mata, D. Stalke, *Angew. Chem. Int. Ed.* **2022**, *16*, e2022036.
3. P. N. Ruth, J. Sarcevic, R. Herbst-Irmer, C. P. Sindlinger, D. Stalke, Angew. Chem. Int. Ed. 2032, 61, e202301609; hot paper.
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5. a) J. Jung, A. Münch, R. Herbst-Irmer, D. Stalke, Angew. Chem. Int. Ed. 2021, 60, 5679-5682;
   b) P. A. M. Stark, L. Kumar, F. Rüttger, K. Rachuy, R. Herbst-Irmer, D. Stalke, Z. Anorg. Allg. Chem. 2024, e202400138.

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